

Weak Separability for Two-way Functional Data: Concept and Test

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Abstract:

This paper concerns multi-way functional data where double or multiple indices are involved. To alleviate the difficulties associated with modeling of the multi-way covariance structure, a commonly used assumption is the separable covariance assumption $C(s, t; u, v) = aC_1(s, u)C_2(t, v)$, which we call *strong separability* in contrast to the *weak separability* that will be introduced in this paper. With the proposed weak separability structure, the covariance can be approximated by a weighted sum of spatial-temporal separable components, including strong separability as a special case. Given a sample of independent realizations of the underlying two-way functional data, we propose tests for the weak separable hypothesis based on the representation using eigenfunctions of the marginal kernels $\int_{\mathcal{T}} C(s, t; u, t)dt$ and $\int_{\mathcal{S}} C(s, t; s, v)ds$. Tests are based on carefully derived asymptotic distributions which are χ^2 type mixtures. The methods are demonstrated by simulations and by an application to mortality data observed for many years over a range of ages, for a sample of countries.

KEYWORDS: separability, spatial-temporal, marginal kernels, tensor product, asymptotic distribution

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1 Introduction

Traditional functional data analysis usually concerns data recorded over a continuum, such as growth curves. Dense and regularly-observed functional data can be recorded in a matrix with dimension $n \times T$, where n is the number of subjects and T is the number of grid points observed for each subject. Two-way functional data refers to an extension where double indices are involved and data can be recorded in a tensor with dimension at least three. Examples include brain imaging data where for each subject $i = 1, \dots, n$, we have $X_i(s, t)$, with a spatial index $s \in \mathbb{R}^d$ and a time index $t \in \mathbb{R}^1$. Other examples include repeatedly or longitudinally observed functional data, such as data obtained from tracking apps where subjects' 24-hour profiles of activities are recorded every day. This type of data can be represented by $X_i(s, t)$, where s denotes the day and t denotes the time within a day.

As two-way functional data becomes more common with modern techniques, the modeling of this type of data attracts increasing interest. Assume the individual observations $X_i(s, t)$ are i.i.d. realizations from an underlying random process $X(s, t)$ in $L^2(\mathcal{S} \times \mathcal{T})$, $s \in \mathcal{S} \subseteq \mathbb{R}^{d_1}$, $t \in \mathcal{T} \subseteq \mathbb{R}^{d_2}$, with mean $\mu(s, t)$ and covariance function $C(s, t; u, v) = \text{cov}(X(s, t), X(u, v))$. Most applications involve modeling of the complex spatial-temporal dependencies, i.e., the structure of $C(s, t; u, v)$. For dense and equally-spaced p grid points in \mathcal{S} and q grid points in \mathcal{T} , the fully nonparametric estimation of the covariance can be achieved by stacking the two-way-index to form a $p \times q$ vector, computing the $pq \times pq$ sample covariance, and reorganizing it back accordingly. However, p and q could both be hundreds or thousands in practice, and the total dimension $pq \times pq$ easily goes beyond the capacity of most data analysis tools. Moreover, the stacking method does not fully bring out the characteristics of the spatial-temporal interactions. Therefore, appropriate structural assumptions on $C(s, t; u, v)$ could be very useful in the estimation and interpretation of large scale two-way functional data.

A commonly used dimension reduction assumption is the separable covariance assumption

$C(s, t; u, v) = aC_1(s, u)C_2(t, v)$, which we call *strong separability* in contrast to the *weak separability* that will be proposed in this paper. There is a large amount of literature on strong separability in related fields (Lu & Zimmerman, 2005; Fuentes, 2006; Srivastava et al., 2009; Hoff et al., 2011; Horváth & Kokoszka, 2012). In functional data analysis settings, we assume that an i.i.d. sample of realizations of the smooth random process $X(s, t)$ are available; therefore, the estimation of separable covariance functions can be done in a non-parametric fashion. Tests for strong separability in functional data settings have been proposed recently (Aston et al., 2015; Constantinou et al., 2015). Factorization of the signal into its spatial (row) and temporal (column) components, with or without explicitly stating the separable covariance assumption, is a common strategy used in many methods in image analysis and two-way functional data analysis (Zhang & Zhou, 2005; Lu et al., 2006; Huang et al., 2009; Chen & Müller, 2012; Hung et al., 2012; Allen et al., 2014; Chen et al., 2017, 2015). Chen et al. (2017) proposed the product FPCA, which looks for dimension reduction of $X_i(s, t)$ using orthogonal basis expansions in the form of $f_j(s)g_k(t)$, where $\{f_j : j \geq 1\}$ and $\{g_k : k \geq 1\}$ are orthogonal bases of $L^2(\mathcal{S})$ and $L^2(\mathcal{T})$, respectively. Despite the empirical success of these factorization methods, the rigorous justification of these methods is still mainly restricted to the scope of strong separability. Under strong separability, the full covariance function factorizes as a product of the spatial covariance function and the temporal covariance function, and their eigenfunctions naturally are the optimal basis functions for the spatial and temporal components in many aspects.

However, the strong separability is a restrictive assumption, as the full separation of spatial and temporal components is unrealistic in many applications. Some non-separable covariance structures are proposed as alternatives in the area of spatial-temporal analysis (Cressie & Huang, 1999; Gneiting, 2002; Stein, 2005; Wikle et al., 2001; Banerjee et al., 2014). These mainly utilize specific parametric assumptions or additional assumptions such as stationarity. In this paper, we will introduce a novel concept of *weak separability*, and propose a statistic

based on the empirical covariance of the estimated marginal projection scores to test the weak separable assumption. We carefully derive the asymptotic null distribution of the test statistic, which is a χ^2 type mixture. Weak separability is a flexible extension of strong separability, and it retains many good properties in the spirit of separability. For example, the covariance $C(s, t; u, v)$ can be approximated by a weighted sum of several strong separable components. The natural basis functions for the factorized spatial and temporal effects are eigenfunctions of the marginal kernels $\int_{\mathcal{T}} C(s, t; u, t) dt$ and $\int_{\mathcal{S}} C(s, t; s, v) ds$, respectively. The eigenfunctions of the full covariance $C(s, t; u, v)$ can be written as tensor products of the marginal eigenfunctions.

The rest of the paper is organized as follows: In Section 2, we introduce the concept of *weak separability* and discuss its properties and applications. In Section 3, we propose an estimation and testing procedure for the assumption of *weak separability*. In Section 4, we illustrate the testing procedure by numerical experiments. In Section 5, we present a data application using a longitudinal mortality dataset, followed by a discussion of further applications of weak separability. Detailed proofs can be found in the appendix.

2 Weak separability: concepts and properties

2.1 Notation

Let H be a real separable Hilbert space, with inner product $\langle \cdot, \cdot \rangle$. Following standard definitions, we denote the space of bounded linear operators on H as $\mathcal{B}(H)$, the space of Hilbert-Schmidt operators on H as $\mathcal{B}_{HS}(H)$, and the space of trace-class operators on H as $\mathcal{B}_{Tr}(H)$. For any trace-class operator $T \in \mathcal{B}_{Tr}(H)$, we define its trace by $Tr(T) = \sum_{i \geq 1} \langle T e_i, e_i \rangle$, where $(e_i)_{i \geq 1}$ is an orthonormal basis of H , and it is easy to see that the definition is independent of the choice of basis.

For H_1 and H_2 two real separable Hilbert spaces, we use \otimes as the standard tensor product, i.e., for $x_1 \in H_1$ and $x_2 \in H_2$, $(x_1 \otimes x_2)$ is the operator from H_2 to H_1 defined by $(x_1 \otimes x_2)y =$

$\langle x_2, y \rangle x_1$ for any $y \in H_2$. With a bit of abuse of notation, we let $H = H_1 \otimes H_2$ denote the tensor product Hilbert space, which contains all finite sums of $x_1 \otimes x_2$, with inner product $\langle x_1 \otimes x_2, y_1 \otimes y_2 \rangle = \langle x_1, y_1 \rangle \langle x_2, y_2 \rangle$, for $x_1, y_1 \in H_1$ and $x_2, y_2 \in H_2$. For $C_1 \in \mathcal{B}(H_1)$ and $C_2 \in \mathcal{B}(H_2)$, we let $C_1 \tilde{\otimes} C_2$ denote the unique bounded linear operator on $H_1 \otimes H_2$ satisfying

$$C_1 \tilde{\otimes} C_2(x_1 \otimes x_2) = C_1 x_1 \otimes C_2 x_2, \quad \text{for all } x_1 \in H_1, x_2 \in H_2.$$

Furthermore, if $C_1 \in \mathcal{B}_{Tr}(H_1)$ and $C_2 \in \mathcal{B}_{Tr}(H_2)$, then $C_1 \tilde{\otimes} C_2 \in \mathcal{B}_{Tr}(H_1 \otimes H_2)$. Following the notation in Aston et al. (2015), we define the partial trace with respect to H_1 as the unique bounded linear operator $Tr_1 : \mathcal{B}_{Tr}(H_1 \otimes H_2) \rightarrow \mathcal{B}_{Tr}(H_2)$, satisfying $Tr_1(C_1 \tilde{\otimes} C_2) = Tr(C_1)C_2$ for all $C_1 \in \mathcal{B}_{Tr}(H_1)$, $C_2 \in \mathcal{B}_{Tr}(H_2)$. The partial trace with respect to H_2 is defined symmetrically and denoted by Tr_2 .

2.2 Two-way functional data and weak separability

For $\mathcal{S} \subseteq \mathbb{R}^{d_1}$ and $\mathcal{T} \subseteq \mathbb{R}^{d_2}$, we consider the space of square integrable surfaces $L^2(\mathcal{S} \times \mathcal{T})$ with the standard inner product, $\langle f, g \rangle = \int_{\mathcal{T}} \int_{\mathcal{S}} f(s, t)g(s, t)dsdt$ and the corresponding norm $\|\cdot\|$. This is a real separable Hilbert space and it is a tensor product space that can be identified with $L^2(\mathcal{S}) \otimes L^2(\mathcal{T})$. Throughout the paper, we focus on $d_1 = d_2 = 1$.

The two-way functional data can be viewed as a random element $X \in L^2(\mathcal{S} \times \mathcal{T})$, and we assume it has well defined mean $\mu = EX$ and covariance operator $C = E[(X - \mu) \otimes (X - \mu)]$. Correspondingly, we denote the mean function by $\mu(s, t) = E(X(s, t))$ and the covariance function by $C(s, t; u, v) = \text{cov}(X(s, t), X(u, v))$, for all $s \in \mathcal{S}$ and $t \in \mathcal{T}$. When we can do so without confusion, we use the same symbol for the covariance operator and its kernel function. We have $C \in B_{HS}(L^2(\mathcal{S} \times \mathcal{T}))$ and $C \in B_{Tr}(L^2(\mathcal{S} \times \mathcal{T}))$. We further define $C_{\mathcal{T}} = Tr_1(C)$ and $C_{\mathcal{S}} = Tr_2(C)$. One can prove that $C_{\mathcal{S}}$ and $C_{\mathcal{T}}$ are HS operators and trace-class operators on $L^2(\mathcal{S})$, and $L^2(\mathcal{T})$, respectively, with symmetric positive definite

kernel functions:

$$C_{\mathcal{S}}(s, u) = \int_{\mathcal{T}} C(s, t; u, t) dt, \quad C_{\mathcal{T}}(t, v) = \int_{\mathcal{S}} C(s, t; s, v) ds. \quad (1)$$

Detailed proofs can be found in Lemma 1 in Chen et al. (2017) and Proposition C.2 in Aston et al. (2015). We call $C_{\mathcal{S}}(s, u)$ and $C_{\mathcal{T}}(t, v)$ the marginal kernel functions hereafter.

For orthogonal bases $\{f_j, j \geq 1\}$ in $L^2(\mathcal{S})$ and $\{g_k, k \geq 1\}$ in $L^2(\mathcal{T})$, the product functions $\{f_j(s)g_k(t), j \geq 1, k \geq 1\}$ form an orthogonal basis of $L^2(\mathcal{S} \times \mathcal{T})$. We can then have

$$X(s, t) = \mu(s, t) + \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \tilde{\chi}_{jk} f_j(s) g_k(t),$$

where $\tilde{\chi}_{jk} = \int_{\mathcal{T}} \int_{\mathcal{S}} (X(s, t) - \mu(s, t)) f_j(s) g_k(t) ds dt$, and then

$$C(s, t; u, v) = \sum_{j, j', k, k'} \text{cov}(\tilde{\chi}_{jk}, \tilde{\chi}_{j'k'}) f_j(s) g_k(t) f_{j'}(u) g_{k'}(v). \quad (2)$$

Definition of weak separability: $X(s, t)$ is weakly separable if there exist orthonormal bases $\{f_j, j \geq 1\}$ and $\{g_k, k \geq 1\}$ such that $\text{cov}(\tilde{\chi}_{jk}, \tilde{\chi}_{j'k'}) = 0$ for $j \neq j'$ or $k \neq k'$, i.e., the scores $\{\tilde{\chi}_{jk}, j \geq 1, k \geq 1\}$ are uncorrelated with each other.

In the following, we list several important properties of weak separability, which make this concept attractive in many applications. Detailed proofs are given in the appendix.

Lemma 1 *If X is weakly separable, the pair of bases $\{f_j, j \geq 1\}$ and $\{g_k, k \geq 1\}$ that satisfies weak separability is unique, and $f_j(s) \equiv \psi_j(s)$ and $g_k(t) \equiv \phi_k(t)$, where $\psi_j(s)$ and $\phi_k(t)$ are the eigenfunctions of the marginal kernels $C_{\mathcal{S}}(s, u)$ and $C_{\mathcal{T}}(t, v)$ as defined in Equation (1). Here the eigen decompositions are $C_{\mathcal{S}}(s, u) = \sum_{j=1}^{\infty} \lambda_j \psi_j(s) \psi_j(u)$ and $C_{\mathcal{T}}(t, v) = \sum_{k=1}^{\infty} \gamma_k \phi_k(t) \phi_k(v)$, where $\lambda_1 \geq \lambda_2 \geq \dots$, and $\gamma_1 \geq \gamma_2 \geq \dots$, are the marginal eigenvalues.*

Lemma 1 allows us to test the weak separability assumption (see Section 3), and we can estimate the spatial and temporal bases through the decomposition of marginal covariance functions.

Lemma 2 *Strong separability defined as $C(s, t; u, v) = aC_1(s, u)C_2(t, v)$ with identifiability constraints $\int_{\mathcal{S}} C_1(s, s)ds = 1$ and $\int_{\mathcal{T}} C_2(t, t)dt = 1$ implies weak separability. And up to a constant scaling, C_1 and C_2 are the same as the marginal kernels.*

Lemma 2 shows that strong separability is a special case of weak separability and the following Lemma 3 further illustrates that weak separability is much more flexible than strong separability.

We define the *marginal projection scores* $\chi_{jk} = \int_{\mathcal{T}} \int_{\mathcal{S}} (X(s, t) - \mu(s, t))\psi_j(s)\phi_k(t)dsdt$, and $\eta_{jk} = \text{var}(\chi_{jk})$. Under weak separability, Equation (2) becomes

$$C(s, t; u, v) = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \eta_{jk} \psi_j(s) \psi_j(u) \phi_k(t) \phi_k(v). \quad (3)$$

Lemma 3 *Let V denote the array $V = (\eta_{jk}, j \geq 1, k \geq 1)$. The strong separability is weak separability with an additional assumption that $\text{rank}(V) = 1$. Moreover, under strong separability $V = a\Lambda\Gamma^T$, where $\Lambda = (\lambda_1, \lambda_2, \dots)^T$ and $\Gamma = (\gamma_1, \gamma_2, \dots)^T$ are the eigenvalues of the marginal kernels, and $a = 1 / \int_{\mathcal{T}} \int_{\mathcal{S}} C(s, t; s, t)dsdt$ is a normalization constant.*

Define *nonnegative rank* $\text{rank}_+(V) = \min\{\ell : V = V_1 + \dots + V_\ell, V_i \geq 0, \text{rank}(V_i) = 1, \forall i\}$, where $V_i \geq 0$ means that V_i is entry-wise nonnegative. Generalizing the above lemma, if $\text{rank}_+(V) = L < \infty$, then V has nonnegative decomposition $V = \sum_{l=1}^L a^l \Lambda^l (\Gamma^l)^T$, where $\Lambda^l = (\lambda_j^l)_{j \geq 1}$ and $\Gamma^l = (\gamma_k^l)_{k \geq 1}$ are all nonnegative for $l = 1, \dots, L$. The constant a^l is for identifiability; for example, one can require $\sum_{j \geq 1} \lambda_j^l = 1$ and $\sum_{k \geq 1} \gamma_k^l = 1$.

Let $C_S^l(s, u) = \sum_j \lambda_j^l \psi_j(s) \psi_j(u)$ and $C_T^l(t, v) = \sum_k \gamma_k^l \phi_k(t) \phi_k(v)$, and then we have

$$L\text{-separability : } C(s, t; u, v) = \sum_{l=1}^L a^l C_S^l(s, u) C_T^l(t, v), \quad (4)$$

where the full covariance function is a sum of L strongly separable components. We can see that $C_S^l(s, u)$ has common eigenfunctions for $l = 1, \dots, L$, which are also eigenfunctions of the marginal kernel $C_S(s, u)$. The case for $C_T^l(t, v)$ is analogous. The strong separability corresponds to 1-separability.

We know that $\text{rank}(V) \leq \text{rank}_+(V)$. In the case of $\text{rank}(V) < \text{rank}_+(V)$, the formulation of the nonnegative-rank decomposition of V is itself a very challenging problem (Lee & Seung, 2001; Donoho & Stodden, 2003; Arora et al., 2012) and is beyond the scope of this paper. We will pursue it in a following piece of work. In practice, we will approximate the spatial effect with P components and the temporal effect with K components. The array $V_{P,K} = (\eta_{jk}, 1 \leq j \leq P, 1 \leq k \leq K)$ often satisfies $\text{rank}(V_{P,K}) = \text{rank}_+(V_{P,K}) = \min(P, K)$, in which case the decomposition of the covariance structure into several strong separable covariances is relatively straightforward. We will illustrate this application in the data analysis in Section 5.

3 Test of weak separability

Assume we have a sample of smooth processes $X_i(s, t) \stackrel{\text{i.i.d.}}{\sim} X(s, t)$, and the marginal projection scores $\chi_{i,jk} = \int_{\mathcal{T}} \int_{\mathcal{S}} (X_i(s, t) - \mu(s, t)) \psi_j(s) \phi_k(t) ds dt$, where $\psi_j(s)$ and $\phi_k(t)$ are the eigenfunctions of marginal covariances. By the definition of weak separability and Lemma 1, the test of weak separability is the same as testing the covariance structure of the marginal projection scores, i.e., $H_0 : \text{cov}(\chi_{jk}, \chi_{j'k'}) = 0$ for $j \neq j'$ or $k \neq k'$.

The problem of testing covariance structure is a classic problem in multivariate analysis.

Suppose we have i.i.d. copies of a p -variate random variable, with mean μ and covariance matrix Σ , and we want to test the null hypothesis that Σ is diagonal. Under the traditional multivariate setting where p is fixed and does not increase with n , likelihood ratio methods can be used to test the diagonality of Σ (Anderson, 1984). Note that these methods require distributional assumptions. The high-dimensional problem has been studied in the context that $p/n \rightarrow \gamma \in (0, \infty)$ or even for p much larger than n (Ledoit & Wolf, 2002; Liu et al., 2008; Cai et al., 2011; Lan et al., 2015). Recently, Chang et al. (2017) applied the wild bootstrap procedure (Chernozhukov et al., 2014) in hypothesis testing for a covariance structure. However, unlike the traditional covariance testing problem, we do not directly observe the sample values $\chi_{i,jk}$. Instead they are estimated from the sample curves $X_i(s, t), i = 1, \dots, n$, as

$$\hat{\chi}_{i,jk} = \int_{\mathcal{T}} \int_{\mathcal{S}} (X_i(s, t) - \bar{X}(s, t)) \hat{\psi}_j(s) \hat{\phi}_k(t) ds dt, \quad (5)$$

where $\bar{X}(s, t) = (1/n) \sum_{i=1}^n X_i(s, t)$ and $\hat{\psi}_j$ and $\hat{\phi}_k$ are eigenfunctions of the estimated marginal covariances, $\hat{C}_{\mathcal{S}}(s, u) = (1/n) \sum_{i=1}^n \int_{\mathcal{T}} (X_i(s, t) - \bar{X}(s, t))(X_i(u, t) - \bar{X}(u, t)) dt$, and $\hat{C}_{\mathcal{T}}(t, v) = (1/n) \sum_{i=1}^n \int_{\mathcal{S}} (X_i(s, t) - \bar{X}(s, t))(X_i(s, v) - \bar{X}(s, v)) ds$. In practice, if the data for each subject are observed on arbitrarily dense and equally spaced grid points and recorded in matrices $X_i, i = 1, \dots, n$, the above estimators can be simplified as $\hat{C}_{\mathcal{S}} = (1/n) \sum_{i=1}^n (X_i - \bar{X})(X_i - \bar{X})^T$, and $\hat{C}_{\mathcal{T}}(t, v) = (1/n) \sum_{i=1}^n (X_i - \bar{X})^T (X_i - \bar{X})$. If we define the sample covariance operator as $C_n = (1/n) \sum_{i=1}^n (X_i - \bar{X}) \otimes (X_i - \bar{X})$, the estimated marginal covariance operators can also be written as $\hat{C}_{\mathcal{S}} = Tr_2(C_n)$ and $\hat{C}_{\mathcal{T}} = Tr_1(C_n)$. We will use these equalities in proofs but not in computation. The estimated marginal covariances are calculated without having to calculate C_n . After obtaining $\hat{C}_{\mathcal{S}}$ and $\hat{C}_{\mathcal{T}}$, one obtains the eigenfunctions $\hat{\phi}_j$ and $\hat{\psi}_k$ by standard eigen-decomposition methods for functional data and estimates the marginal scores by numerical approximations of the integrals (Chen et al., 2017). Although we can prove that the $\hat{\chi}_{i,jk}$ are \sqrt{n} -consistent estimators of the $\chi_{i,jk}$, most test statistics based on $\hat{\chi}_{i,jk}$ have different null distributions from their counterparts using

$\chi_{i,jk}$, and this prevents us from directly using the above-mentioned testing procedures.

3.1 The test statistic and its properties

For $j \neq j'$ and/or $k \neq k'$, define

$$T_n(j, k, j', k') = \frac{1}{\sqrt{n}} \sum_{i=1}^n \hat{\chi}_{i,jk} \hat{\chi}_{i,j'k'}. \quad (6)$$

Condition I: For some orthonormal basis $(e_j)_{j \geq 1}$ of $L^2(\mathcal{S} \times \mathcal{T})$, $\sum_j (\mathbb{E}(\langle X, e_j \rangle^4))^{1/4} < \infty$.

Condition II: For some integers P and K , we have $\delta_P = \min_{1 \leq j \leq P} (\lambda_j - \lambda_{j+1}) > 0$ and $\delta_K = \min_{1 \leq k \leq K} (\gamma_k - \gamma_{k+1}) > 0$.

Remark: (Mas, 2006; Aston et al., 2015) Condition I implies $\mathbb{E}\|X\|^4 < \infty$. Under $\mathbb{E}\|X\|^4 < \infty$, we have $\sqrt{n}(C_n - C)$ converges to a Gaussian random element in $B_{HS}(L^2(\mathcal{S} \times \mathcal{T}))$. Under Condition I, we have a stronger form of convergence such that $\sqrt{n}(C_n - C)$ converges to a Gaussian random element in $B_{Tr}(L^2(\mathcal{S} \times \mathcal{T}))$.

Theorem 4 *Under Condition I, we have $\mathcal{Z} = \sqrt{n}(C_n - C)$ converges to a Gaussian random element in $B_{Tr}(L^2(\mathcal{S} \times \mathcal{T}))$. For $1 \leq j, j' \leq P$ and $1 \leq k, k' \leq K$ as defined in Condition II, if X is weak separable, we have*

(i) for $j \neq j'$ and $k \neq k'$,

$$T_n(j, k, j', k') = \text{Tr} \left(((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_{k'})) \mathcal{Z} \right) + o_p(1),$$

(ii) for $j = j'$ and $k \neq k'$,

$$\begin{aligned} T_n(j, k, j, k') &= \text{Tr} \left(((\psi_j \otimes \psi_j) \tilde{\otimes} (\phi_k \otimes \phi_{k'})) \mathcal{Z} \right) \\ &\quad + \text{Tr} \left((Id_1 \tilde{\otimes} (\eta_{jk'}(\gamma_k - \gamma_{k'})^{-1} \phi_k \otimes \phi_{k'})) \mathcal{Z} \right) \\ &\quad + \text{Tr} \left((Id_1 \tilde{\otimes} (\eta_{jk}(\gamma_{k'} - \gamma_k)^{-1} \phi_{k'} \otimes \phi_k)) \mathcal{Z} \right) + o_p(1), \end{aligned}$$

(iii) for $j \neq j'$ and $k = k'$,

$$\begin{aligned} T_n(j, k, j', k) &= \text{Tr} \left(((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_k)) \mathcal{Z} \right) \\ &\quad + \text{Tr} \left(((\eta_{jk}(\lambda_{j'} - \lambda_j)^{-1} \psi_{j'} \otimes \psi_j) \tilde{\otimes} Id_2) \mathcal{Z} \right) \\ &\quad + \text{Tr} \left(((\eta_{j'k}(\lambda_j - \lambda_{j'})^{-1} \psi_j \otimes \psi_{j'}) \tilde{\otimes} Id_2) \mathcal{Z} \right) + o_p(1), \end{aligned}$$

where Id_1 and Id_2 are identity operators on $L^2(\mathcal{S})$ and $L^2(\mathcal{T})$, respectively.

Remark: Since $\sqrt{n} \text{Tr} \left(((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_{k'})) C \right)$ is zero under the null hypothesis, the first term is the same as $\sqrt{n} \text{Tr} \left(((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_{k'})) C_n \right) = \frac{1}{\sqrt{n}} \sum_i \chi_{i,jk} \chi_{i,j'k'}$, i.e., the counterpart of T_n as if we have the true marginal projection scores. The second and third terms, if they exist, are the non-negligible estimation errors.

Corollary 5 *Under the conditions of Theorem 4, if X is weak separable, for different sets of (j, k, j', k') , satisfying $1 \leq j, j' \leq P$, $1 \leq k, k' \leq K$, and $(j, k) \neq (j', k')$, the $T_n(j, k, j', k')$'s are asymptotically jointly Gaussian with mean zero and covariance structure Γ . The formula of Γ is given in the proof.*

3.2 Tests based on χ^2 type mixtures

Lemma 6 *For $j \neq j'$, $\sum_k \mathbb{E}(\chi_{jk} \chi_{j'k}) = 0$, and for $k \neq k'$, $\sum_j \mathbb{E}(\chi_{jk} \chi_{jk'}) = 0$. This also holds in the empirical version such that for $j \neq j'$, $\sum_k T_n(j, k, j', k) = 0$, and for $k \neq k'$, $\sum_j T_n(j, k, j, k') = 0$.*

Recall the fact that principal component scores in traditional functional principal component analysis are uncorrelated. This lemma is a generalized result for the marginal projection scores in two-way functional data.

Due to this linear relationship between the different terms of T_n , the statistic we consider is the sum of squares of the terms of T_n without normalizing by the covariance. In practice, for suitably chosen P_n and K_n , we use the statistic defined as

$$S_n = \sum_{1 \leq j, j' \leq P_n, 1 \leq k, k' \leq K_n, (j, k) < (j', k')} (T_n(j, k, j', k'))^2, \quad (7)$$

where $(j, k) < (j', k')$ means $(j - 1) * K_n + k < (j' - 1) * K_n + k'$. This is used due to the symmetry $T_n(j, k, j', k') = T_n(j', k', j, k)$, so that we only include the “upper diagonal” part of the cross covariance among the marginal scores.

Take T_n to be a long vector of length $d = P_n K_n (P_n K_n - 1)/2$ created by stacking all of the $T_n(j, k, j', k')$, $1 \leq j, j' \leq P_n$, $1 \leq k, k' \leq K_n$, $(j, k) < (j', k')$. Then by Corollary 5, $T_n \sim N_d(0, \Gamma)$ under H_0 , where we now take Γ to be a covariance matrix. Define the spectral decomposition of Γ as $\Gamma = U \Sigma U^T$, where Σ is diagonal with diagonal entries $\sigma_1, \dots, \sigma_d$ which are the eigenvalues of Γ , ordered from largest to smallest, and $U = [u_1 \ u_2 \ \dots \ u_d]$ where the u_i are orthonormal column vectors. By Lemma 6, Γ is degenerate, so some of the σ_i are 0. Since $S_n = \|T_n\|^2 = \|U^T T_n\|^2$ and $U^T T_n \sim N_d(0, \Sigma)$, we can write $S_n = \sum_{i=1}^d \sigma_i A_i$ where the A_i are i.i.d. χ_1^2 , i.e., the null distribution of S_n is a weighted sum of χ^2 distributions, which we call a χ^2 type mixture.

The Welch-Satterthwaite approximation for a χ^2 type mixture (Zhang, 2013) approximates $S_n \sim \beta \chi_d^2$ and determines β and d from matching the first 2 cumulants (the mean and the variance). This results in $\beta = \text{var}(S_n)/(2\text{E}(S_n)) = \text{Tr}(\Gamma^2)/\text{Tr}(\Gamma)$ and $d = 2(\text{E}(S_n))^2/\text{var}(S_n) = (\text{Tr}(\Gamma))^2/\text{Tr}(\Gamma^2)$. By using a plug in estimator of Γ , we can approximate the P-value for our test as an upper tail probability of $\beta \chi_d^2$. When the first (P_n, K_n) terms do not satisfy weak

separability, we have $S_n \xrightarrow{P} \infty$, by noticing that for at least one set of (j, k, j', k') , the first term in Equation (14) (in the proof of Theorem 4) is on the order of \sqrt{n} .

A criterion we will use to evaluate a given choice of P_n and K_n is the “fraction of variance explained” (FVE) by the first P_n and K_n components, defined as

$$\text{FVE}(P_n, K_n) = \frac{\frac{1}{n} \sum_{i=1}^n \sum_{j=1}^{P_n} \sum_{k=1}^{K_n} \hat{\chi}_{i,jk}^2}{\frac{1}{n} \sum_{i=1}^n \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \hat{\chi}_{i,jk}^2}. \quad (8)$$

This definition can be justified by noting its relation to the normalized mean squared L^2 loss of the truncated data $\tilde{X}_i(s, t) = \mu(s, t) + \sum_{j=1}^{P_n} \sum_{k=1}^{K_n} \chi_{i,jk} \psi_j(s) \phi_k(t)$. In particular,

$$\frac{\frac{1}{n} \sum_{i=1}^n \int_{\mathcal{T}} \int_{\mathcal{S}} (X_i(s, t) - \tilde{X}_i(s, t))^2 \psi_j(s) \phi_k(t) ds dt}{\frac{1}{n} \sum_{i=1}^n \int_{\mathcal{T}} \int_{\mathcal{S}} (X_i(s, t) - \mu(s, t))^2 \psi_j(s) \phi_k(t) ds dt} = 1 - \frac{\frac{1}{n} \sum_{i=1}^n \sum_{j=1}^{P_n} \sum_{k=1}^{K_n} \chi_{i,jk}^2}{\frac{1}{n} \sum_{i=1}^n \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \chi_{i,jk}^2}.$$

The latter term is approximated by our definition of FVE. The above equality only relies on the orthogonality of the eigenfunctions, not the weak separability assumptions. Thus, it still makes sense to consider this definition of FVE even when H_0 is not true.

We also define the “marginal FVE’s” $\text{FVE}_S(P_n) = \sum_{j=1}^{P_n} \hat{\lambda}_j / \sum_{j=1}^{\infty} \hat{\lambda}_j$ and $\text{FVE}_T(K_n) = \sum_{k=1}^{K_n} \hat{\gamma}_k / \sum_{k=1}^{\infty} \hat{\gamma}_k$, where the $\hat{\lambda}_j$ are the eigenvalues of \hat{C}_S and the $\hat{\gamma}_k$ are the eigenvalues of \hat{C}_T . Note that in practice the infinite sums in the denominators of $\text{FVE}(P_n, K_n)$, $\text{FVE}_S(P_n)$, and $\text{FVE}_T(K_n)$ will have to be replaced with the largest number of terms that can reasonably be considered nonzero.

Noting that $\sum_j \text{E} \chi_{jk}^2 = \gamma_k$, $\sum_k \text{E} \chi_{jk}^2 = \lambda_j$ and $\sum_{j,k} \text{E} \chi_{jk}^2 = \sum_j \lambda_j = \sum_k \gamma_k$, we have

$$\text{FVE}(P_n, K_n) \gtrsim \text{FVE}_S(P_n) + \text{FVE}_T(K_n) - 1,$$

subject to estimation error (to see, for example, that $\sum_k \text{E} \chi_{jk}^2 = \lambda_j$, take $j = j'$ in the proof of Lemma 6). Therefore, we propose the following rule of thumb to choose P_n and K_n : First

choose P_n and K_n such that the marginal FVE's are at least 90%. If this choice results in $\text{FVE}(P_n, K_n) \geq 90\%$, use these values of P_n and K_n . If not, use the values of P_n and K_n that have marginal FVE's at least 95%, in which case $\text{FVE}(P_n, K_n)$ is expected to be above 90%.

3.3 Bootstrap approximation

As an alternative to asymptotic approximation, we can also consider a bootstrap approach to approximate the distribution of the test statistic. Theorem 4 provides theoretical support for the use of the following empirical bootstrap procedure and parametric bootstrap procedure (Van Der Vaart & Wellner, 1996). Our simulations show that the asymptotic approximation based on the χ^2 type mixture has very satisfactory performance and appears to be superior to the bootstrap approximation. We still present the bootstrap approximation here since it is generally applicable to similar tests where the asymptotic null distributions do not have closed form.

Empirical bootstrap: At each step, draw a random sample from the data X_1, \dots, X_n with replacement. Denote this sample as X_1^*, \dots, X_n^* . Let

$$\hat{\chi}_{i,jk}^* = \int_{\mathcal{T}} \int_{\mathcal{S}} (X_i^*(s, t) - \bar{X}^*(s, t)) \hat{\psi}_j^*(s) \hat{\phi}_k^*(t) ds dt, \quad (9)$$

where \bar{X}^* is the sample mean of the X_i^* , and the $\hat{\psi}_j^*$ and $\hat{\phi}_k^*$ are the eigenfunctions of the estimated marginal covariances of the X_i^* . The signs of the $\hat{\psi}_j^*$ and $\hat{\phi}_k^*$ are chosen to minimize $\|\hat{\psi}_j^* - \hat{\psi}_j\|$ and $\|\hat{\phi}_k^* - \hat{\phi}_k\|$, respectively. Let

$$T_n^*(j, k, j', k') = \frac{1}{\sqrt{n}} \sum_{i=1}^n \hat{\chi}_{i,jk}^* \hat{\chi}_{i,j'k'}^*. \quad (10)$$

The empirical bootstrap test statistic is calculated as

$$S_n^* = \sum_{1 \leq j, j' \leq P_n, 1 \leq k, k' \leq K_n, (j, k) < (j', k')} (T_n^*(j, k, j', k') - T_n(j, k, j', k'))^2.$$

This procedure is repeated B times, and the P-value is approximated as the proportion of bootstrap test statistics S_n^* that are larger than the test statistic S_n .

Validity: Theorem 3.9.13 in Van Der Vaart & Wellner (1996) can be used to prove the validity of the bootstrap procedure, i.e., the conditional random laws (given data) of S_n^* are asymptotically consistent almost surely for estimating the laws of S_n , under the null hypothesis. By Theorem 4, we have that under the null hypothesis, T_n can be written as $\Phi'_P(\sqrt{n}(\mathcal{P}_n - P)) + o(1)$ and $T_n^* - T_n$ can be written as $\Phi'_P(\sqrt{n}(\mathcal{P}_n^* - \mathcal{P}_n)) + o(1)$, where Φ'_P is a linear continuous mapping that depends on the three different cases in Theorem 4. Thus, Theorem 3.9.13 applies.

Parametric bootstrap: While the empirical bootstrap procedure requires no distributional assumptions on X , the parametric bootstrap procedure assumes $X \sim F(\mu, C)$; that is, we know the distribution of X up to its mean μ and covariance operator C . Usually, F is taken to be normal. We perform the parametric bootstrap procedure as follows: At each step, generate independent $\chi_{i,jk}^* \sim F(0, \frac{1}{n} \sum_{i'=1}^n \hat{\chi}_{i',jk}^2)$ and then define $X_i^*(s, t) = \bar{X}(s, t) + \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \chi_{i,jk}^* \hat{\psi}_j(s) \hat{\phi}_k(t)$. In practice, the infinite sums will have to be replaced with the largest number of terms that can reasonably be considered nonzero. Note that, conditional on the data X_1, \dots, X_n , the X_i^* 's have a weak separable covariance structure. Calculate the $\hat{\chi}_{i,jk}^*$ and $T_n^*(j, k, j', k')$ as in Equation (9) and Equation (10). The parametric bootstrap test statistic is calculated as

$$S_n^* = \sum_{1 \leq j, j' \leq P_n, 1 \leq k, k' \leq K_n, (j, k) < (j', k')} (T_n^*(j, k, j', k'))^2.$$

This procedure is repeated B times, and the P-value is approximated as the proportion of bootstrap test statistics S_n^* that are larger than the test statistic S_n .

4 Numerical study

To numerically evaluate our test of weak separability for finite sample sizes, we perform the test on simulated data. We first consider data of the form $X_i(s, t) = \sum_{j=1}^3 \sum_{k=1}^3 \chi_{i,jk} \psi_j(s) \phi_k(t)$, $i = 1, \dots, n$, where the scores $\chi_{i,jk}$ are mean 0 random variables that we generate directly. We let s and t take values from 0 to 1 on an evenly spaced grid of 20 points. We use ψ_j as the Fourier series basis functions $\psi_1(s) = -\sqrt{2}\cos(2\pi s)$, $\psi_2(s) = \sqrt{2}\sin(2\pi s)$, and $\psi_3(s) = -\sqrt{2}\cos(4\pi s)$. We define the ϕ_k as the first 3 B-spline basis functions produced by Matlab's "spcol" function, using order 4, with knots at 0, .5, and 1. We then normalize the sets of ψ_j and ϕ_k .

The $\chi_{i,jk}$ are generated as follows: Define a 3×3 nonnegative matrix $V = (\eta_{jk} : 1 \leq j, k \leq 3)$. We generate each matrix $\chi_i = (\chi_{i,jk} : 1 \leq j, k \leq 3)$ independently from a specified distribution with $\text{var}(\chi_{i,jk}) = \eta_{jk}$ and $\text{cov}(\chi_{i,jk}, \chi_{i,j'k'}) = 0$ for all $(j, k) < (j', k')$ except for $\text{cov}(\chi_{i,12}, \chi_{i,21}) = c$, where c is some constant. $c = 0$ indicates that H_0 is true, while $|c| > 0$ indicates that H_0 is violated, and H_0 is violated to a larger degree for larger $|c|$. As an alternate method to produce data under the alternative hypothesis, we also consider a covariance structure with $\text{cov}(\chi_{i,11}, \chi_{i,12}) = b$, $\text{cov}(\chi_{i,21}, \chi_{i,22}) = -3b/4$, and $\text{cov}(\chi_{i,31}, \chi_{i,32}) = -b/4$, where b is some constant. Note that these covariance terms satisfy Lemma 6.

We consider two different choices of the distribution of the χ_i . The first is the multivariate normal $N(0, \Sigma)$. Here, Σ is a 9×9 matrix whose diagonal values are from V as described above (see below for the exact values of V that are considered), and whose off-diagonal values are controlled by c and b . The second is the multivariate t distribution. To simulate a multivariate t -distributed vector of length p with covariance matrix Σ and degrees of freedom

v , we first simulate a length- p vector x from the multivariate normal distribution with mean 0 and covariance matrix Σ . One standard definition of a multivariate t vector is $x/\sqrt{u/v}$, where u is chi-square random variable with v degrees of freedom that is independent of x . However, to make the covariance matrix of the multivariate t vector equal to Σ , we use $x/\sqrt{u/(v-2)}$ as our multivariate t vector. We take $v = 6$ in our simulations.

We consider two different choices of V , which we will denote as V_1 and V_2 . We define them as follows:

$$V_1 = \begin{bmatrix} 0.6652 \\ 0.2447 \\ 0.0900 \end{bmatrix} \begin{bmatrix} 0.7856 & 0.1753 & 0.0391 \end{bmatrix} = \begin{bmatrix} 0.5226 & 0.1166 & 0.0260 \\ 0.1923 & 0.0429 & 0.0096 \\ 0.0707 & 0.0158 & 0.0035 \end{bmatrix},$$

$$V_2 = \begin{bmatrix} 1 & 0 \\ 0 & .6 \\ 0 & .4 \end{bmatrix} \begin{bmatrix} .6652 & .2447 & .0900 \\ .7856 & .1753 & .0391 \end{bmatrix} = \begin{bmatrix} 0.6652 & 0.2447 & 0.0900 \\ 0.4714 & 0.1052 & 0.0235 \\ 0.3142 & 0.0701 & 0.0156 \end{bmatrix}.$$

When $c = b = 0$, V_1 corresponds to a strong separable covariance structure, while V_2 corresponds to a weak separable covariance structure that is not strong separable (see Lemma 3). Using V_1 and $c = b = 0$, the leading eigenvalues of the marginal covariances C_S and C_T are (0.6652, 0.2447, 0.0900) and (0.7856, 0.1753, 0.0391), respectively. Using V_2 and $c = b = 0$, the leading eigenvalues of the marginal covariances C_S and C_T are (1.0000, 0.6000, 0.4000) and (1.4508, 0.4200, 0.1291), respectively. To study power, for a given choice of V_1 or V_2 , we take c to be the largest positive value, rounded down to the nearest hundredth, such that Σ is positive definite. This value is .14 for V_1 and .33 for V_2 . We also do simulations with c taken to be half of these values. Additionally, we do power simulations where b is chosen as the largest positive value, rounded down to the nearest hundredth, such that Σ is positive definite, as well as half of this value.

For each of 200 trials, we simulate data $X_i(s, t)$, $i = 1, \dots, n$, in the manner described above. We consider both $n = 100$ and $n = 500$. We estimate the marginal projection scores, calculate the test statistic, and obtain P-values from the test procedures as described in Section 3, using $B = 1000$ for the bootstrap procedures. The rejection rates for the different scenarios described above are shown in Tables 1 and 2. We chose P_n and K_n using the FVE-based rule of thumb described in Section 3. Most trials ended up with $P_n = 3$ and $K_n = 2$.

Table 1: Rejection rates for the weak separability test procedures using V_1 . “ χ^2 ” denotes the χ^2 type mixture approximation which estimates the full covariance Γ , “Emp” denotes the empirical bootstrap, and “Para” denotes the parametric bootstrap.

Scenario		n=100			n=500		
		χ^2	Emp	Para	χ^2	Emp	Para
Normal	$c = 0, b = 0$	0.035	0.040	0.050	0.050	0.060	0.065
	$c = .07, b = 0$	0.975	0.970	0.985	1	1	1
	$c = .14, b = 0$	1	1	1	1	1	1
	$c = 0, b = .06$	0.990	0.990	0.995	1	1	1
	$c = 0, b = .12$	1	1	1	1	1	1
Multi-variate t	$c = 0, b = 0$	0.015	0.015	0.225	0.040	0.025	0.395
	$c = .07, b = 0$	0.745	0.670	0.985	0.995	0.995	1
	$c = .14, b = 0$	1	0.985	1	1	1	1
	$c = 0, b = .06$	0.830	0.755	0.995	1	0.995	1
	$c = 0, b = .12$	1	0.970	1	1	1	1

From Table 1 and Table 2, we can see that the χ^2 type mixture approximation performs the best. It is able to control the Type-I errors under all scenarios and achieves very good power as n , c , and b increase. The empirical bootstrap procedure seems slightly conservative and less powerful. The parametric bootstrap performs well for normal data, but it is invalid for multivariate t data. Therefore, we recommend to use the test based on the χ^2 type mixture approximation developed in Section 3.2.

As an alternative simulation method, we generate the data X_i , $i = 1, \dots, n$, i.i.d. directly from a distribution with mean 0 and covariance structure C , defined as follows:

Table 2: Rejection rates for the weak separability test procedures using V_2 . “ χ^2 ” denotes the χ^2 type mixture approximation which estimates the full covariance Γ , “Emp” denotes the empirical bootstrap, and “Para” denotes the parametric bootstrap.

Scenario		n=100			n=500		
		χ^2	Emp	Para	χ^2	Emp	Para
Normal	$c = 0, b = 0$	0.055	0.010	0.090	0.035	0.040	0.045
	$c = .165, b = 0$	0.960	0.690	0.995	1	1	1
	$c = .33, b = 0$	1	0.905	1	1	1	1
	$c = 0, b = .145$	0.990	0.760	0.995	1	1	1
	$c = 0, b = .29$	1	0.865	1	1	1	1
Multi-variate t	$c = 0, b = 0$	0.020	0	0.345	0.030	0.015	0.445
	$c = .165, b = 0$	0.700	0.250	0.980	1	0.980	1
	$c = .33, b = 0$	0.985	0.695	1	1	1	1
	$c = 0, b = .145$	0.785	0.325	0.985	0.995	0.955	1
	$c = 0, b = .29$	0.945	0.620	1	1	0.960	1

$$C(s, t; u, v) = \frac{1}{(t - v)^2 + 1} \exp \left(-\frac{(s - u)^2}{(t - v)^2 + 1} \right) \quad (11)$$

This covariance structure is taken from Example 1 in Gneiting (2002). It is a stationary covariance structure, meaning it depends only on the differences $s - u$ and $t - v$, and it is not strongly separable. Gneiting (2002) suggests covariance structures of this type to model space-time data, for example those pertaining to environmental factors such as wind speed. This covariance structure is also used by Aston et al. (2015) in their simulations as an example of a non-strong separable covariance structure.

As before, we let s and t take values from 0 to 1 on an evenly spaced grid of 20 points. For 200 trials we simulate data $X_i(s, t)$, $i = 1, \dots, n$, from either multivariate normal or multivariate t and perform the test. Table 3 shows the simulation results. The rejection rates (excluding the parametric bootstrap procedure for multivariate t data, which has already been shown to be invalid in this case) are near or below .05, suggesting that this covariance structure, though not strong separable, is weak separable. Using the FVE-based rule of thumb described in

Section 3, most trials in these simulations ended up with $P_n = 2$ and $K_n = 2$.

Table 3: Rejection rates for the weak separability test procedures using the covariance structure from Equation (11). “ χ^2 ” denotes the χ^2 type mixture approximation which estimates the full covariance Γ , “Emp” denotes the empirical bootstrap, and “Para” denotes the parametric bootstrap.

Scenario	n=100			n=500		
	χ^2	Emp	Para	χ^2	Emp	Para
Normal	0.045	0.055	0.060	0.050	0.035	0.045
Multivariate t	0.020	0.050	0.215	0.025	0.035	0.210

We visualize a few slices of $C(s, t; u, v)$ from Equation (11) in Figure 1 and compare these to the weak separable approximation $\hat{C}(s, t; u, v) = \sum_{j=1}^2 \sum_{k=1}^2 (\frac{1}{n} \sum_{i=1}^n \hat{\chi}_{i,jk}^2) \hat{\psi}_j(s) \hat{\psi}_j(u) \hat{\phi}_k(t) \hat{\phi}_k(v)$, which is also plotted in Figure 1. Here, the estimated eigenfunctions and scores were obtained from a sample $X_i(s, t)$, $i = 1, \dots, 500$, that were generated i.i.d. normal with mean 0 and covariance structure C , with s and t taking values from 0 to 1 on an evenly spaced grid of 100 points. We see that $C(s, t; u, v)$ and $\hat{C}(s, t; u, v)$ are fairly similar, supporting the results of the test of weak separability.

5 Data application

We apply our test of weak separability to a longitudinal mortality dataset, which has previously been discussed in Chen & Müller (2012). The data are obtained from the Human Mortality Database (www.mortality.org; Wilmoth et al. (2007)). The data consist of period lifetables from different countries. These lifetables show mortality rates across age for a specific period of time, giving surfaces of the form $X_i(s, t)$, $i = 1, \dots, n$, where $X_i(s, t)$ denotes the mortality rate of country i in calendar year t for subjects of age s . $n = 27$ countries were considered, and we assume the data from these countries to be independent. Each country in the dataset has mortality rates measured on the same equally spaced grid, where t takes

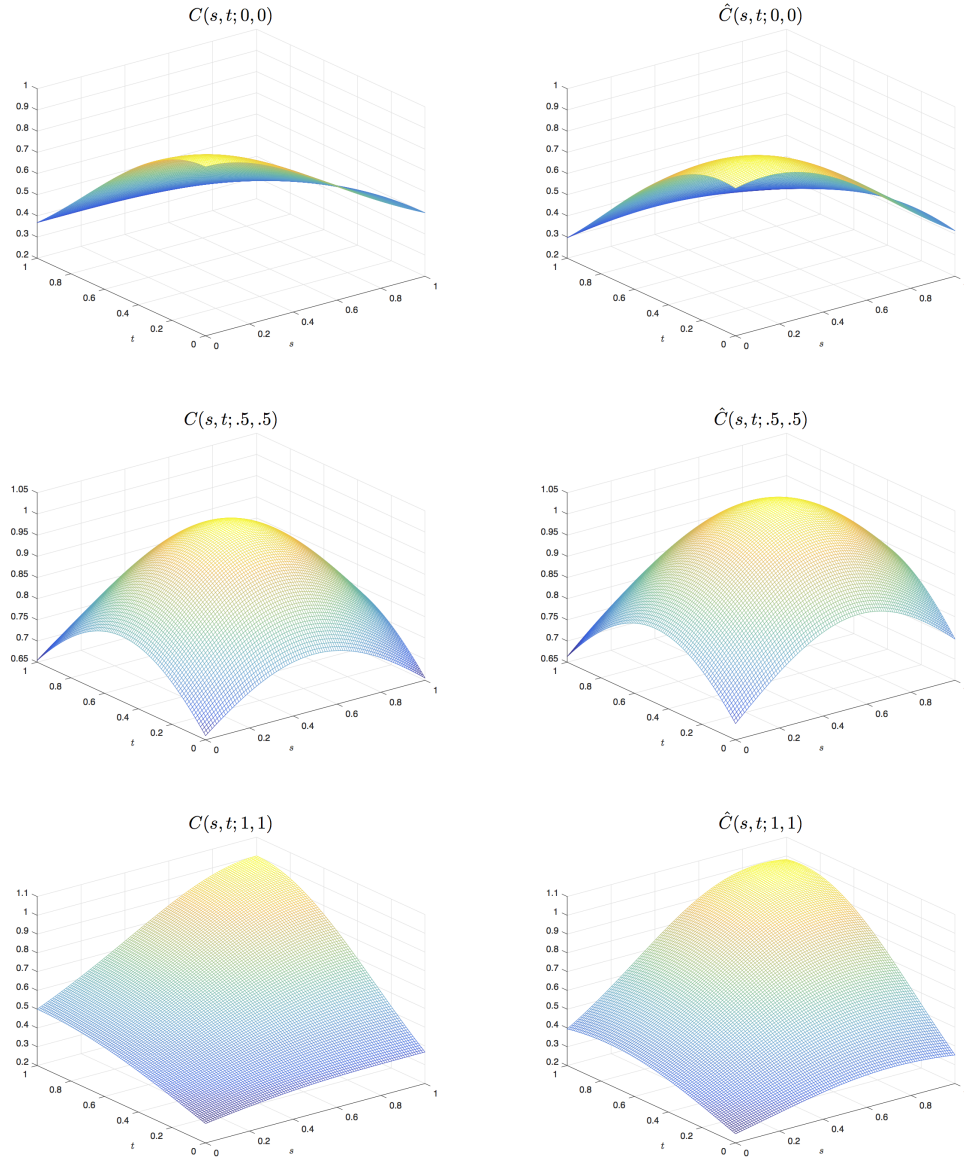


Figure 1: Plots of $C(s, t; u, v)$ and $\hat{C}(s, t; u, v)$ for fixed values of u and v , where C is the covariance structure from Equation (11).

integer values from 1960 to 2006, and s takes integer values from 60 to 100 (chosen since the interest is on death rates of older individuals). Mortality rates tend to increase with age and decrease with year.

The covariance structure $C(s, t; u, v)$ is of interest in studying changes in mortality over age and year, and also is essential in subsequent modeling and analysis such as functional PCA and regression. Note that C has dimension $41 \times 47 \times 41 \times 47$, resulting in about 3.7×10^6 entries. Direct nonparametric estimation of C and visualization of C may be challenging. Looking to represent C with a separable structure, we apply our test of weak separability to the dataset using the procedures from Section 3.2. The values of P_n and K_n are selected to be $P_n = 2$ and $K_n = 4$ by the FVE procedure described in Section 3.2, which gives $\text{FVE}(P_n, K_n) = 0.9102$. We obtain a P-value of 0.6498, and fail to reject H_0 , indicating that we may assume the data to have a weak separable covariance structure.

We also apply the test of strong separability proposed by Aston et al. (2015) to this dataset via their R package “covsep” (Tavakoli, 2016). Recall that, by Lemma 3, strong separability corresponds to $\eta_{jk} = a\lambda_j\gamma_k$. We use their empirical bootstrap test function with $B = 1000$ and no studentization to get a P-value for each η_{jk} , $j = 1, 2$, $k = 1, \dots, 4$. We obtain the P-values (0.001, 0.004, 0.003, 0.002; 0.000, 0.009, 0.013, 0.014). Since all these P-values are low, we can conclude that the strong separability test from Aston et al. (2015) rejects strong separability for the dataset.

In general, following Equation (3) and Equation (4), we can approximate a weak separable covariance structure $C(s, t; u, v)$ with $P_n = 2$ and $K_n = 4$ as

$$\begin{aligned}
\hat{C}(s, t; u, v) &= \sum_{j=1}^2 \sum_{k=1}^4 \hat{\eta}_{jk} \hat{\psi}_j(s) \hat{\psi}_j(u) \hat{\phi}_k(t) \hat{\phi}_k(v) \\
&= \left(\sum_{k=1}^4 \hat{\eta}_{1k} \right) \hat{\psi}_1(s) \hat{\psi}_1(u) \sum_{k=1}^4 \frac{\hat{\eta}_{1k}}{\sum_{k'=1}^4 \hat{\eta}_{1k'}} \hat{\phi}_k(t) \hat{\phi}_k(v) \\
&\quad + \left(\sum_{k=1}^4 \hat{\eta}_{2k} \right) \hat{\psi}_2(s) \hat{\psi}_2(u) \sum_{k=1}^4 \frac{\hat{\eta}_{2k}}{\sum_{k'=1}^4 \hat{\eta}_{2k'}} \hat{\phi}_k(t) \hat{\phi}_k(v) \\
&= a^1 \hat{C}_S^1(s, u) \hat{C}_T^1(t, v) + a^2 \hat{C}_S^2(s, u) \hat{C}_T^2(t, v)
\end{aligned} \tag{12}$$

We see that we can decompose $C(s, t; u, v)$ into 2 strong separable terms. These are plotted for the mortality dataset in Figure 2. Here, \hat{C}_T^1 and \hat{C}_T^2 are complicated but have a similar structure, being positive with a peak near the middle of the range of years. We see from \hat{C}_S^1 and \hat{C}_S^2 that there is little covariance between mortality rates for low values of age. The values of \hat{C}_S^1 are all positive, while \hat{C}_S^2 gives a negative contribution to the covariance between mortality rates for low and high ages.

If we had strong separability, the covariance between mortality rates in years t and v would be the same, regardless of age, up to a constant, where the constant would depend on the ages of interest s and u . By contrast, our decomposition above says that the covariance between mortality rates in years t and v is a weighted sum of two covariance structures, where the weights depend on the ages of interest s and u . An analogous statement can be made for the covariance between mortality rates for two ages s and u .

It is natural to ask if the decomposition given in Equation (12) is in any sense unique or optimal. Consider the case when V_{P_n, K_n} has full rank and $P_n \leq K_n$. Then $\text{rank}_+(V_{P_n, K_n}) = P_n$, and we can have the non-negative rank-one decomposition $V_{P_n, K_n} = \sum_{l=1}^{P_n} a^l \Lambda^l (\Gamma^l)^T$, where $\Lambda^l = (\lambda_j^l)_{1 \leq j \leq P_n}$ and $\Gamma^l = (\gamma_k^l)_{1 \leq k \leq K_n}$, and we define $C_S^l = \sum_{j=1}^{P_n} \lambda_j^l \psi_j(s) \psi_j(u)$ and $C_T^l = \sum_{k=1}^{K_n} \gamma_k^l \phi_k(t) \phi_k(v)$ (see Section 2). We require $\sum_j \lambda_j^l = 1$ and $\sum_k \gamma_k^l = 1$. In general,

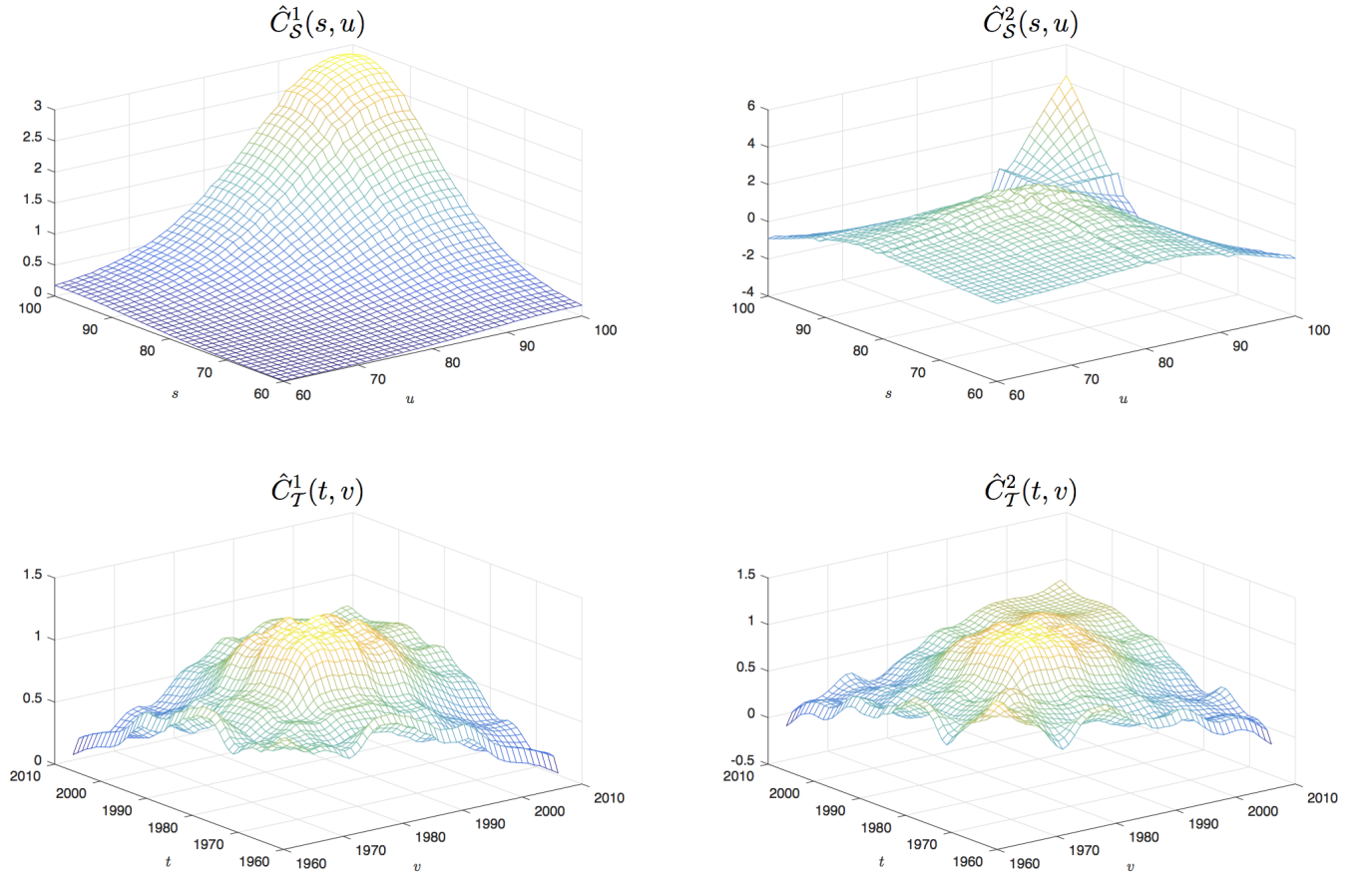


Figure 2: Plot of the components of the decomposition of $C(s,t;u,v)$. To improve visibility, slight smoothing was done on \hat{C}_T^1 and \hat{C}_T^2 .

there are many possible choices for this non-negative rank-one decomposition. If one imposes the condition that Λ^j is orthogonal to Λ^l for $1 \leq j < l \leq P_n$, then the decomposition of V_{P_n, K_n} is unique (Ding et al., 2006). The unique decomposition under the above conditions is given by Λ^l being the l th column of the identity matrix I_{P_n} , and $a^l \Gamma^l$ being the l th row of V_{P_n, K_n} . In our data application, this leads to the unique decomposition in Equation (12). Interestingly, with the orthogonality condition, we can also identify this decomposition with a decomposition of the truncated original process, writing $\tilde{X}(s, t) = \sum_{l=1}^{P_n} \tilde{X}_l(s, t)$, where $\tilde{X}_l(s, t) = \sum_{k=1}^{K_n} \chi_{lk} \psi_l(s) \phi_k(t)$. Under weak separability, the χ_{jk} are uncorrelated, and hence the \tilde{X}_l are uncorrelated. Additionally, each \tilde{X}_l has the strong separable covariance structure $C_S^l(s, u) C_T^l(t, v)$. Hence, our covariance decomposition lends itself to a simple interpretation, being the sum of covariances of uncorrelated processes. Note that if we had $P_n > K_n$, we could make an analogous decomposition using the transpose of V_{P_n, K_n} in place of V_{P_n, K_n} . General properties of decompositions based on L -separability, especially when V does not have full rank, will be the focus of an upcoming work.

6 Appendix: proofs

Proof of Lemma 1

Let $(f_j)_{j \geq 1}$ and $(g_k)_{k \geq 1}$ be a pair of bases that satisfy weak separability. Under weak separability, Equation (2) becomes

$$C(s, t; u, v) = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \text{var}(\tilde{\chi}_{jk}) f_j(s) g_k(t) f_j(u) g_k(v).$$

Under the condition that $E\|X\|^4 < \infty$, the first marginal kernel can be written

$$\begin{aligned} C_S(s, u) &= \int_{\mathcal{T}} \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \text{var}(\tilde{\chi}_{jk}) f_j(s) g_k(t) f_j(u) g_k(t) dt \\ &= \sum_{j=1}^{\infty} \left(\sum_{k=1}^{\infty} \text{var}(\tilde{\chi}_{jk}) \right) f_j(s) f_j(u). \end{aligned}$$

We see that the f_j are eigenfunctions of C_S with eigenvalues $\lambda_j = \sum_{k=1}^{\infty} \text{var}(\tilde{\chi}_{jk})$. An analogous computation shows that the g_k are eigenfunctions of $C_{\mathcal{T}}$ with eigenvalues $\gamma_k = \sum_{j=1}^{\infty} \text{var}(\tilde{\chi}_{jk})$.

Proof of Lemma 2

With strong separability, we have $C(s, t; u, v) = aC_1(s, u)C_2(t, v)$. From the definition of C_S we have

$$C_S(s, u) = \int_{\mathcal{T}} C(s, t; u, t) dt = aC_1(s, u) \int_{\mathcal{T}} C_2(t, t) dt = aC_1(s, u).$$

An analogous argument shows $C_{\mathcal{T}}(t, v) = aC_2(t, v)$. Note that $a = \int_{\mathcal{T}} \int_{\mathcal{S}} C(s, t; s, t) ds dt$.

Thus we have

$$C(s, t; u, v) = \frac{1}{a} C_S(s, u) C_{\mathcal{T}}(t, v) = \frac{1}{a} \sum_{j=1}^{\infty} \lambda_j \psi_j(s) \psi_j(u) \sum_{k=1}^{\infty} \gamma_k \phi_k(t) \phi_k(v).$$

Therefore,

$$\begin{aligned} \text{cov}(\chi_{jk}, \chi_{j'k'}) &= \int_{\mathcal{T}, \mathcal{S}, \mathcal{T}, \mathcal{S}} C(s, t; u, v) \psi_j(s) \phi_k(t) \psi_{j'}(u) \phi_{k'}(v) ds dt du dv \\ &= \frac{1}{a} \sum_{j^*=1}^{\infty} \sum_{k^*=1}^{\infty} \lambda_{j^*} \gamma_{k^*} U_{j^*j} U_{j^*j'} W_{k^*k} W_{k^*k'}, \end{aligned} \tag{13}$$

where we define $U_{jj'} = \int_{\mathcal{S}} \psi_j(s) \psi_{j'}(s) ds$ and $W_{kk'} = \int_{\mathcal{T}} \phi_k(t) \phi_{k'}(t) dt$. When $j \neq j'$ or $k \neq k'$, we see that at least one of U_{j^*j} , $U_{j^*j'}$, W_{k^*k} , or $W_{k^*k'}$ will be 0 regardless of the values of j^*

and k^* . Thus, $\text{cov}(\chi_{jk}, \chi_{j'k'}) = 0$, and we have weak separability.

Proof of Lemma 3

Since V is of rank 1, V can be written $V = WZ^T$, where W and Z are column vectors with entries (w_1, w_2, \dots) and (z_1, z_2, \dots) , respectively. Thus, $\eta_{jk} = w_j z_k$, and Equation (3) can be written

$$\begin{aligned} C(s, t; u, v) &= \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} w_j z_k \psi_j(s) \psi_j(u) \phi_k(t) \phi_k(v) \\ &= \left(\sum_{j=1}^{\infty} w_j \psi_j(s) \psi_j(u) \right) \left(\sum_{k=1}^{\infty} z_k \phi_k(t) \phi_k(v) \right). \end{aligned}$$

The above can be normalized to fit the definition of strong separability in Lemma 2.

Further, using Equation (13) with $j = j'$ and $k = k'$, we get $\eta_{jk} = \frac{1}{\int_{\mathcal{T}} \int_{\mathcal{S}} C(s, t; s, t) ds dt} \lambda_j \gamma_k$, so $V = \frac{1}{\int_{\mathcal{T}} \int_{\mathcal{S}} C(s, t; s, t) ds dt} \Lambda \Gamma^T$. Note that the normalization constant is $a = \frac{1}{\int_{\mathcal{T}} \int_{\mathcal{S}} C(s, t; s, t) ds dt}$.

Proof of Theorem 4

From Condition 1 in Section 3.1 and the remark following it,

$$\sqrt{n}(C_n - C) \xrightarrow{d} N(0, \Sigma_C),$$

where we define $\Sigma_C = E(((X - \mu) \otimes (X - \mu) - C) \tilde{\otimes} ((X - \mu) \otimes (X - \mu) - C))$. Using the notation in Section 2,

$$T_n(j, k, j', k') = \sqrt{n} \langle C_n(\hat{\psi}_j \otimes \hat{\phi}_k), \hat{\psi}_{j'} \otimes \hat{\phi}_{k'} \rangle = \sqrt{n} \text{Tr}((\hat{\psi}_j \otimes \hat{\psi}_{j'}) \tilde{\otimes} (\hat{\phi}_k \otimes \hat{\phi}_{k'}) C_n).$$

Using (5.1.8) in Hsing & Eubank (2015), we have

$$(\hat{\psi}_j - \psi_j) = \mathcal{M}_j(\hat{C}_S - C_S) \psi_j + o_p(\hat{\psi}_j - \psi_j),$$

where $\mathcal{M}_j = \sum_{m \neq j} (\lambda_j - \lambda_m)^{-1} \psi_m \otimes \psi_m \in B_{Tr}(\mathcal{S})$ and λ_j is the j th eigenvalue of $C_{\mathcal{S}}$. Analogously,

$$(\hat{\phi}_k - \phi_k) = \mathcal{M}'_k (\hat{C}_{\mathcal{T}} - C_{\mathcal{T}}) \phi_k + o_p(\hat{\phi}_k - \phi_k),$$

where $\mathcal{M}'_k = \sum_{m \neq k} (\gamma_k - \gamma_m)^{-1} \phi_m \otimes \phi_m \in B_{Tr}(\mathcal{S})$ and γ_k is the k th eigenfunction of $C_{\mathcal{T}}$.

Using $\hat{C}_{\mathcal{S}} - C_{\mathcal{S}} = Tr_2(C_n - C)$ and $\hat{C}_{\mathcal{T}} - C_{\mathcal{T}} = Tr_1(C_n - C)$, we can write $T_n(j, k, j', k')$ as

$$\begin{aligned} T_n(j, k, j', k') = & \sqrt{n} Tr \left((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_{k'}) C \right) \\ & + \sqrt{n} Tr \left((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_{k'}) (C_n - C) \right) \\ & + \sqrt{n} Tr \left((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes (\mathcal{M}'_{k'} Tr_1(C_n - C) \phi_{k'})) C \right) \\ & + \sqrt{n} Tr \left((\psi_j \otimes \psi_{j'}) \tilde{\otimes} ((\mathcal{M}'_k Tr_1(C_n - C) \phi_k) \otimes \phi_{k'}) C \right) \\ & + \sqrt{n} Tr \left((\psi_j \otimes (\mathcal{M}_{j'} Tr_2(C_n - C) \psi_{j'})) \tilde{\otimes} (\phi_k \otimes \phi_{k'}) C \right) \\ & + \sqrt{n} Tr \left((\mathcal{M}_j Tr_2(C_n - C) \psi_j) \otimes \psi_{j'} \tilde{\otimes} (\phi_k \otimes \phi_{k'}) C \right) \\ & + o_p(1). \end{aligned} \tag{14}$$

Note that the first term in the above equation is zero under H_0 . Under H_0 , we have the representation $C(s, t, u, v) = \sum_{j,k} \eta_{jk} \psi_j(s) \psi_j(u) \phi_k(t) \phi_k(v)$, where $\eta_{jk} = \text{var}(\chi_{jk})$. Also, by Proposition C.1 in Aston et al. (2015), we have that $Tr(ATr_1(T)) = Tr((Id_1 \tilde{\otimes} A)T)$, where Id_1 is an identity operator on \mathcal{S} , $A \in B(\mathcal{T})$, and $T \in B_{Tr}(\mathcal{S} \times \mathcal{T})$. An analogous identity holds for $Tr_2(T)$. Using these facts, along with $\mathcal{Z} = \sqrt{n}(C_n - C)$, we give a simplified form of $T_n(j, k, j', k')$ under H_0 for 3 cases:

Case (i) $j \neq j'$ and $k \neq k'$:

$$T_n(j, k, j', k') = Tr \left(((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_{k'})) \mathcal{Z} \right) + o_p(1).$$

Case (ii) $j = j'$ and $k \neq k'$:

$$\begin{aligned} T_n(j, k, j', k') &= \text{Tr} \left(((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_{k'})) \mathcal{Z} \right) \\ &\quad + \text{Tr} \left((Id_1 \tilde{\otimes} (\eta_{jk'}(\phi_k \otimes \phi_{k'}) \mathcal{M}'_k)) \mathcal{Z} \right) \\ &\quad + \text{Tr} \left((Id_1 \tilde{\otimes} (\eta_{jk}(\phi_{k'} \otimes \phi_k) \mathcal{M}'_{k'})) \mathcal{Z} \right) + o_p(1). \end{aligned}$$

Case (iii) $j \neq j'$ and $k = k'$:

$$\begin{aligned} T_n(j, k, j', k') &= \text{Tr} \left(((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_{k'})) \mathcal{Z} \right) \\ &\quad \text{Tr} \left(((\eta_{jk}(\psi_{j'} \otimes \psi_j) \mathcal{M}_{j'}) \tilde{\otimes} Id_2) \mathcal{Z} \right) \\ &\quad + \text{Tr} \left(((\eta_{j'k}(\psi_j \otimes \psi_{j'}) \mathcal{M}_j) \tilde{\otimes} Id_2) \mathcal{Z} \right) + o_p(1). \end{aligned}$$

In each of the above cases, two or more of the terms in Equation (14) end up being zero due to the orthogonality of the eigenfunctions. The latter 2 cases can be simplified to get the result in the statement of the theorem by noting that, for Case (ii), $\eta_{jk'}(\phi_k \otimes \phi_{k'}) \mathcal{M}'_k = \eta_{jk'}(\gamma_k - \gamma_{k'})^{-1} \phi_k \otimes \phi_{k'}$ and $\eta_{jk}(\phi_{k'} \otimes \phi_k) \mathcal{M}'_{k'} = \eta_{jk}(\gamma_{k'} - \gamma_k)^{-1} \phi_{k'} \otimes \phi_k$, and for Case (iii), $\eta_{jk}(\psi_{j'} \otimes \psi_j) \mathcal{M}_{j'} = \eta_{jk}(\lambda_{j'} - \lambda_j)^{-1} \psi_{j'} \otimes \psi_j$ and $\eta_{j'k}(\psi_j \otimes \psi_{j'}) \mathcal{M}_j = \eta_{j'k}(\lambda_j - \lambda_{j'})^{-1} \psi_j \otimes \psi_{j'}$.

Proof of Corollary 5

From Theorem 4, we can see that all the terms of $T_n(j, k, j', k')$ can be written in the form $\text{Tr}(A_1 \tilde{\otimes} A_2 \mathcal{Z})$ for some $A_1 \in B(\mathcal{S})$ and $A_2 \in B(\mathcal{T})$. Since \mathcal{Z} converges to a Gaussian random element and $\text{Tr}(A_1 \tilde{\otimes} A_2 \mathcal{Z})$ is a continuous linear mapping, the $T_n(j, k, j', k')$ are Gaussian, and they are jointly Gaussian for different sets of (j, k, j', k') . Denote $T_n(j, k, j', k') \xrightarrow{d} N(0, \gamma(j, k, j', k'))$, and let Γ be the covariance structure of the joint distribution of the $T_n(j, k, j', k')$. The $\gamma(j, k, j', k')$ and Γ can be calculated from terms of the form

$$\mathbb{E}(\text{Tr}(A_1 \tilde{\otimes} A_2 \mathcal{Z}) \text{Tr}(B_1 \tilde{\otimes} B_2 \mathcal{Z})) = \text{Tr} \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right),$$

where Σ_C is defined as in the proof of Theorem 4.

Recall the K-L expansion of the process $X(s, t) = \mu(s, t) + \sum_{j,k} \chi_{jk} \psi_j(s) \phi_k(t)$. We define $u_{ij} = \psi_i \otimes \psi_j \in B_{HS}(\mathcal{S})$, $v_{ij} = \phi_i \otimes \phi_j \in B_{HS}(\mathcal{T})$, $\beta_{ii'jj'kk'll'} = \mathbb{E}[\chi_{ii'} \chi_{jj'} \chi_{kk'} \chi_{ll'}]$ and $\alpha_{ii'} = \mathbb{E}(\chi_{ii'}^2)$. Following the calculations in Appendix B of Aston et al. (2015), we have

$$\begin{aligned} & \text{Tr} \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) \\ &= \sum_{i,i',j,j',k,k',l,l'} \beta_{i,i',j,j',k,k',l,l'} \text{Tr}[A_1 u_{ij}] \text{Tr}[A_2 v_{i'j'}] \text{Tr}[B_1 u_{kl}] \text{Tr}[B_2 v_{k'l'}] \\ &\quad - \sum_{i,i',j,j'} \alpha_{ii'} \alpha_{jj'} \text{Tr}[A_1 u_{ii}] \text{Tr}[B_1 u_{jj}] \text{Tr}[A_2 v_{i'i'}] \text{Tr}[B_2 v_{j'j'}]. \end{aligned} \quad (15)$$

Each of the trace terms in the above equation can be evaluated using the identities $\text{Tr}[Id_1 u_{ij}] = I(i = j)$, $\text{Tr}[Id_2 v_{i'j'}] = I(i' = j')$, $\text{Tr}[(\psi_{j_1} \otimes \psi_{j'_1}) u_{ij}] = I(i = j_1) I(j = j'_1)$, and $\text{Tr}[(\phi_{k_1} \otimes \phi_{k'_1}) v_{i'j'}] = I(i' = k_1) I(j' = k'_1)$. From these identities and the possible forms of A_1 , A_2 , B_1 , and B_2 given in Theorem 4, it follows that the second sum is always 0. The first sum can be simplified by considering 9 cases, as follows:

Case (1) $A_1 = a_1 \psi_{j_1} \otimes \psi_{j'_1}$, $A_2 = a_2 \phi_{k_1} \otimes \phi_{k'_1}$, $B_1 = b_1 \psi_{j_2} \otimes \psi_{j'_2}$, $B_2 = b_2 \phi_{k_2} \otimes \phi_{k'_2}$:

$$\text{Tr} \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) = a_1 a_2 b_1 b_2 \beta_{j_1, k_1, j'_1, k'_1, j_2, k_2, j'_2, k'_2}.$$

Case (2) $A_1 = Id_1$, $A_2 = a_2 \phi_{k_1} \otimes \phi_{k'_1}$, $B_1 = b_1 \psi_{j_2} \otimes \psi_{j'_2}$, $B_2 = b_2 \phi_{k_2} \otimes \phi_{k'_2}$:

$$\text{Tr} \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) = a_2 b_1 b_2 \sum_i \beta_{i, k_1, i, k'_1, j_2, k_2, j'_2, k'_2}.$$

Case (3) $A_1 = a_1 \psi_{j_1} \otimes \psi_{j'_1}$, $A_2 = Id_2$, $B_1 = b_1 \psi_{j_2} \otimes \psi_{j'_2}$, $B_2 = b_2 \phi_{k_2} \otimes \phi_{k'_2}$:

$$\text{Tr} \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) = a_1 b_1 b_2 \sum_{i'} \beta_{j_1, i', j'_1, i', j_2, k_2, j'_2, k'_2}.$$

Case (4) $A_1 = a_1\psi_{j_1} \otimes \psi_{j'_1}$, $A_2 = a_2\phi_{k_1} \otimes \phi_{k'_1}$, $B_1 = Id_1$, $B_2 = b_2\phi_{k_2} \otimes \phi_{k'_2}$:

$$Tr \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) = a_1 a_2 b_2 \sum_k \beta_{j_1, k_1, j'_1, k'_1, k, k_2, k, k'_2}.$$

Case (5) $A_1 = a_1\psi_{j_1} \otimes \psi_{j'_1}$, $A_2 = a_2\phi_{k_1} \otimes \phi_{k'_1}$, $B_1 = b_1\psi_{j_2} \otimes \psi_{j'_2}$, $B_2 = Id_2$:

$$Tr \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) = a_1 a_2 b_1 \sum_{k'} \beta_{j_1, k_1, j'_1, k'_1, j_2, k', j'_2, k'}.$$

Case (6) $A_1 = Id_1$, $A_2 = a_2\phi_{k_1} \otimes \phi_{k'_1}$, $B_1 = Id_1$, $B_2 = b_2\phi_{k_2} \otimes \phi_{k'_2}$:

$$Tr \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) = a_2 b_2 \sum_i \sum_k \beta_{i, k_1, i, k'_1, k, k_2, k, k'_2}.$$

Case (7) $A_1 = Id_1$, $A_2 = a_2\phi_{k_1} \otimes \phi_{k'_1}$, $B_1 = b_1\psi_{j_2} \otimes \psi_{j'_2}$, $B_2 = Id_2$:

$$Tr \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) = a_2 b_1 \sum_i \sum_{k'} \beta_{i, k_1, i, k'_1, j_2, k', j'_2, k'}.$$

Case (8) $A_1 = a_1\psi_{j_1} \otimes \psi_{j'_1}$, $A_2 = Id_2$, $B_1 = Id_1$, $B_2 = b_2\phi_{k_2} \otimes \phi_{k'_2}$:

$$Tr \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) = a_1 b_2 \sum_{i'} \sum_k \beta_{j_1, i', j'_1, i', k, k_2, k, k'_2}.$$

Case (9) $A_1 = a_1\psi_{j_1} \otimes \psi_{j'_1}$, $A_2 = Id_2$, $B_1 = b_1\psi_{j_2} \otimes \psi_{j'_2}$, $B_2 = Id_2$:

$$Tr \left((A_1 \tilde{\otimes} A_2) \widetilde{\bigotimes} (B_1 \tilde{\otimes} B_2) \Sigma_C \right) = a_1 b_1 \sum_{i'} \sum_{k'} \beta_{j_1, i', j'_1, i', j_2, k', j'_2, k'}.$$

In the above, a_1 , a_2 , b_1 , and b_2 are scalar constants. Using the above, all the terms in $\Gamma(j, j', k, k', l, l', m, m')$ can be obtained from straightforward but tedious calculations.

Proof of Lemma 6

When $j \neq j'$,

$$\begin{aligned}
\sum_k \text{cov}(\chi_{jk}, \chi_{j'k}) &= \sum_k \text{Tr} \left((\psi_j \otimes \psi_{j'}) \tilde{\otimes} (\phi_k \otimes \phi_k) C \right) \\
&= \text{Tr} \left((\psi_j \otimes \psi_{j'}) \tilde{\otimes} \left(\sum_k \phi_k \otimes \phi_k \right) C \right) \\
&= \text{Tr} \left(((\psi_j \otimes \psi_{j'}) \tilde{\otimes} Id_2) C \right) \\
&= \text{Tr} \left((\psi_j \otimes \psi_{j'}) \text{Tr}_2(C) \right) \\
&= \text{Tr} \left((\psi_j \otimes \psi_{j'}) C_S \right) = 0.
\end{aligned}$$

The equality $\sum_k \phi_k \otimes \phi_k = Id_2$ follows from the fact that the $(\phi_k)_{k \geq 1}$ are orthogonal basis functions. The last equality follows from the fact that the $(\psi_j)_{j \geq 1}$ are eigenfunctions of the marginal covariance C_S . The same argument holds for the empirical version as follows:

$$\begin{aligned}
\sum_k T_n(j, k, j', k) &= \sum_k \sqrt{n} \text{Tr} \left((\hat{\psi}_j \otimes \hat{\psi}_{j'}) \tilde{\otimes} (\hat{\phi}_k \otimes \hat{\phi}_k) C_n \right) \\
&= \sqrt{n} \text{Tr} \left((\hat{\psi}_j \otimes \hat{\psi}_{j'}) \tilde{\otimes} \left(\sum_k \hat{\phi}_k \otimes \hat{\phi}_k \right) C_n \right) \\
&= \sqrt{n} \text{Tr} \left(((\hat{\psi}_j \otimes \hat{\psi}_{j'}) \tilde{\otimes} Id_2) C_n \right) \\
&= \sqrt{n} \text{Tr} \left((\hat{\psi}_j \otimes \hat{\psi}_{j'}) \text{Tr}_2(C_n) \right) \\
&= \sqrt{n} \text{Tr} \left((\hat{\psi}_j \otimes \hat{\psi}_{j'}) \hat{C}_S \right) = 0.
\end{aligned}$$

Analogous calculations can be done when $k \neq k'$ to show that $\sum_j \text{cov}(\chi_{jk}, \chi_{jk'}) = 0$ and $\sum_j T_n(j, k, j, k') = 0$.

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